## Catalyst Development for Hydroliquefaction of Coal

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## Abstract

This paper summarizes observations made during the development of a catalyst screening test in the initial phases of a program which has as its objective the development of improved catalysts for the direct hydroliquefaction of coal.

The test is carried out batchwise in a stirred autoclave and employs Illinois #6 coal and a commercial petroleum based solvent (Panasol AN3). Uncertainties in reaction time and temperature are normally encountered in this mode of operation due to substantial coal conversions during heating and cooling. These uncertainties have been reduced significantly by injecting coal after a slurry of solvent and catalyst has reached operating temperature and by rapid cooling at the termination of the reaction period.

Products are separated into benzene insoluble, pentane insoluble (asphaltene) and pentane soluble (oil) fractions. Data obtained with a commercial CoMo catalyst in a study of the effect of reaction variables on hydrogen consumption, coal conversion, asphaltene and oil yields, and sulfur removal indicate the following:

Hydrogen absorption is linear with time and continues after maximum coal conversion (93%) is reached. It is also linear with pressure in the range investigated (760-3000 psi) indicating a process first order in hydrogen and therefore independent of coal conversion which becomes zero order in hydrogen above 2000 psi.

A clearcut distinction between first and zero order dependence on coal in the 50-80% conversion range cannot be made. The reaction tends toward first order at higher conversion levels. Substantial conversion of coal is observed in the absence of catalyst and at very short reaction times.

Asphaltene yields are proportional to conversion until about 80% conversion and remain relatively constant thereafter. Oil yields increase with conversion to maximum conversion (93%).

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Sulfur levels in asphaltene and oil decline with increasing yields of these fractions.

The relationship between asphaltene and oil yields and sulfur contents is not affected by temperature or catalyst loading.

Most of these observations can be rationalized via a model in which the major role of catalyst is to maintain the solvent in a suitable state of hydrogenation. Moreover, the data support a branching mechanism for formation of asphaltenes and oil rather than the generally assumed sequence of first order reactions.